

SIMCA®

Application Note

How to turn process data into information

10 June 2020

Introduction

Massive amounts of data are generated every day, both in production plants and development labs. This data is an invaluable source of information that has the potential to be used to gain increased knowledge of processes. In addition to gaining a better understanding of normal process behavior this data will also allow detailed comparison of produced batches as well as fault identification in relation with process upsets. To analyze these data, powerful techniques are required which can manage the special properties of batch process data. The Umetrics Suite is designed to fulfill these criteria by combining proven technologies with state-of-the-art features. SIMCA efficiently analyzes and visualizes data from batch processes while SIMCA-online can propagate this valuable information in real-time for monitoring, prediction, and control purposes. SIMCA-online offers a client server technology where process information is displayed on screen and in real-time for comparison of produced batches or for fault identification in relation with process upsets.

Multivariate Batch Process Modeling

Multivariate Batch process modeling transforms process data into interpretable plots representing a concentration of the original information. A typical example is shown in figures 1 and 2. From the raw data in figure 1, it is a challenge to visually analyze the data, determine normal process variations, or compare batches and assess if they have been processed in a similar or dissimilar way. After analysis in SIMCA, figure 2 displays every batch as one single line over time and it is straightforward to see if the processes were run in a similar way and during which parts of the process there is most variation.

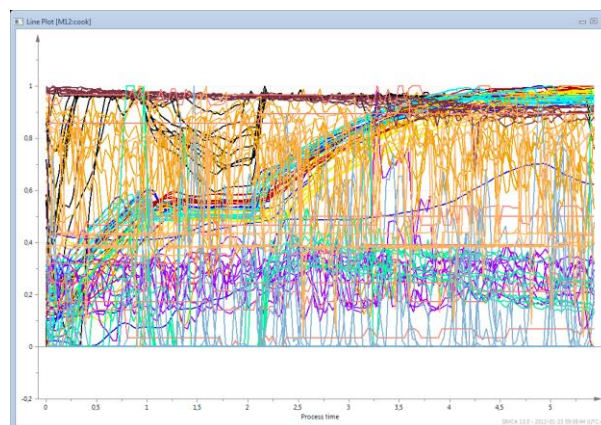


Figure 1: Raw data from 20 batches for which 12 variables have been measured during the process evolution.

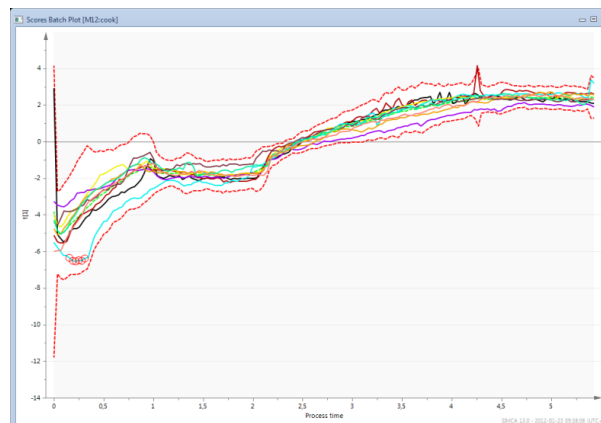


Figure 2: The same data after analysis in SIMCA 13.

One batch in figure 2 shows a different behavior early in the process. The convenient “drill-down” feature in SIMCA creates a Contribution plot of the batch with a simple mouse click, revealing in which variables and how this batch is different from the others in figure 3. By double clicking on a variable in the contribution plot the raw data plot for that variable is produced, figure 4. This quickly provides exact information and simplifies interpretation.

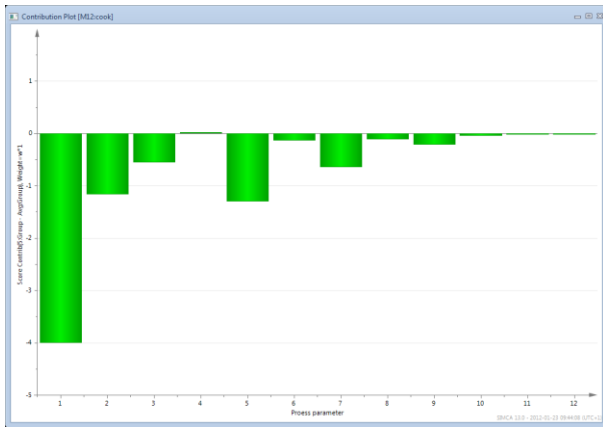


Figure 3: The Contribution plot reveals a different behavior for this batch in many of the modeled variables. All variables show a negative contribution, meaning that they are lower than for the average batch.

Multivariate batch modeling is applicable to many objectives including process diagnostics. For this purpose, a model representing normal process behavior is built. Such a model is a powerful tool in real time process monitoring using SIMCA-online where process deviations are identified, analyzed, and acted upon using the same technology as SIMCA.

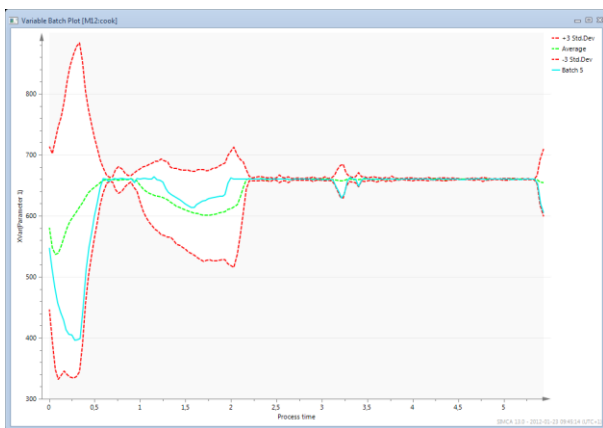


Figure 4: A mouse click on a bar in the variable plot shows the raw data plot for that variable allowing full drill down and straightforward interpretation.

The quality of the resulting product is affected by both starting conditions for the batch (i.e. raw materials, process set points, etc.) as well as influences during process evolution.

Therefore, batch process data is modeled in two stages to allow an overview and supervision of the evolution of the batch as well as a complete summary of all data belonging to one batch. In the second stage, data is reorganized so that each batch is represented by one single point in a plot, instead of a complete line representing the behavior over time as in figure 2. In figure 5, a summary analysis is shown where similar

batches are close to each other and dissimilar ones far apart. This overview allows investigation of time trends in the process between batches, comparison between scales, sites, campaigns, etc. With a mouse-click, the similarities, and differences between two batches or sets of batches is visualized in a single time resolved Contribution plot. This clearly shows which variables are different between batches, how and during which period of the batch lifetime. The relationship between variables, and how these change during the batch, can also be studied using this plot as shown in figure 6.

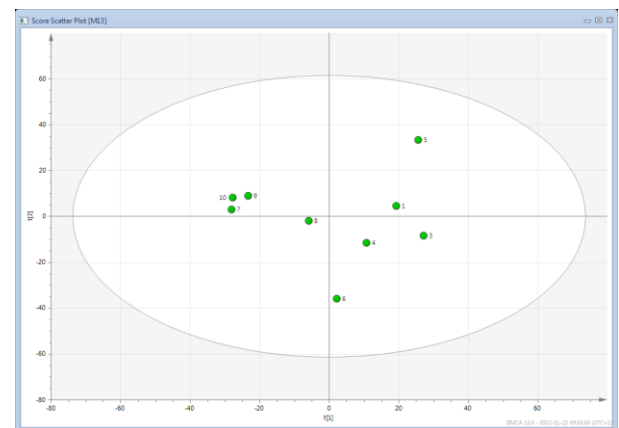


Figure 5: Summary of all batches in one single plot allows straightforward comparison of batches, campaigns, sites, etc. The farther away points are from each other, the more different the batches are. The way in which batches differ can be investigated.

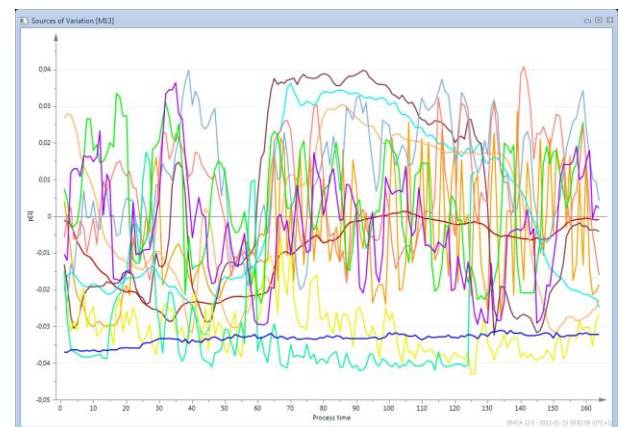


Figure 6: The variable influences are shown in a time resolved figure.

As all data (online, offline, starting conditions and quality) for one batch is collected in one single place; the reason for variations in product quality or throughput can be easily combined and analyzed.

Maximum value from the powerful analysis tools in SIMCA is achieved when the multivariate models are applied in a real-time monitoring system. SIMCA-online tools support production to ensure that processes are

always optimized such that products meet specification and quality goals.

Multivariate Batch process modeling in SIMCA

- Process evolution modeling and monitoring
- Deviation analysis through drill-down root cause inspection
- Analysis of time trends in production
- Batch-to-batch, campaign-to-campaign, site-to-site comparisons
- Analysis of process influence on product